

Coarse graining Nuclear Interactions *

R. Navarro Pérez, J.E. Amaro and E. Ruiz Arriola
Departamento de Física Atómica, Molecular y Nuclear,
Universidad de Granada, E-18071 Granada, Spain.

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Abstract

We consider a coarse graining of NN interactions in coordinate space very much in the spirit of the well known V_{lowk} approach. To this end we sample the interaction at about the minimal de Broglie wavelength probed by NN scattering below pion production threshold. This amounts to provide a simple delta-shell potential plus the standard OPE potential above 2 fm. The possible simplifications in the Nuclear many body problem are discussed.

1 Introduction

The NN interaction provides a basic building block of atomic nuclei. A milestone in the development of the field was achieved when the Nijmegen group generated a fit via a partial wave analysis (PWA) to a set of about 4000 NN scattering data with $\chi^2/\text{dof} \lesssim 1$ [1] after charge dependence (CD) effects were incorporated and discarding about further 1000 of 3σ inconsistent data. The analysis was carried out using an energy dependent potential for which nuclear structure calculations become hard to formulate. Thus, energy independent *high quality* potentials were produced with almost identical χ^2/dof [2, 3]. Among them, the AV18 potential is directly useful for *ab initio* Monte Carlo calculations up to $A = 10$ [4]. While all these potentials differ in their form, in the last years it has been realized that if CM momenta above $\Lambda = 400\text{MeV}$ are explicitly integrated out, the remaining effective interaction has appealing features. The so-called V_{lowk} potentials [5] exhibit an astonishing degree of universality, produce a rather smooth interaction and weaken the strength of the interaction so that Hartree-Fock calculations may be reliable starting points for nuclear structure calculations. In the present talk we address a suitable formulation of the problem in configuration space.

Regardless of these successes it is to date unclear what is the impact of NN uncertainties on finite nuclei due to our ignorance on short distances. Relevant length scales are a) The mean interparticle separation distance $d = 1.8\text{fm}$ as obtained from Nuclear matter saturation density $\rho_0 = 1/d^3 = 0.17\text{fm}^{-3}$, b) The Fermi momentum $k_F = (3/2)^{1/3}/d \sim 250\text{MeV}$ which gives a wavelength of about $\hbar/k_F = 0.8\text{fm}$, c) Minimal relative CM de Broglie wavelength corresponding to the pion production threshold $\lambda = \hbar/\sqrt{M_N m_\pi} \sim 0.5\text{fm}$ and d) The pion Compton wavelength $1/m_\pi = 1.4\text{fm}$. The situation is presented pictorially in Fig. 1 suggesting that for the description of the ground state in light nuclei both the short distance core and the role of explicit pions become marginal. This was recognized long ago [6] where the bulk of ^3He and ^4He could be described with a pionless and soft-core potential which just reproduced the S-wave phase shifts up to $E_{\text{LAB}} \leq 100\text{MeV}$. Actually, we expect this feature to hold for light nuclei.

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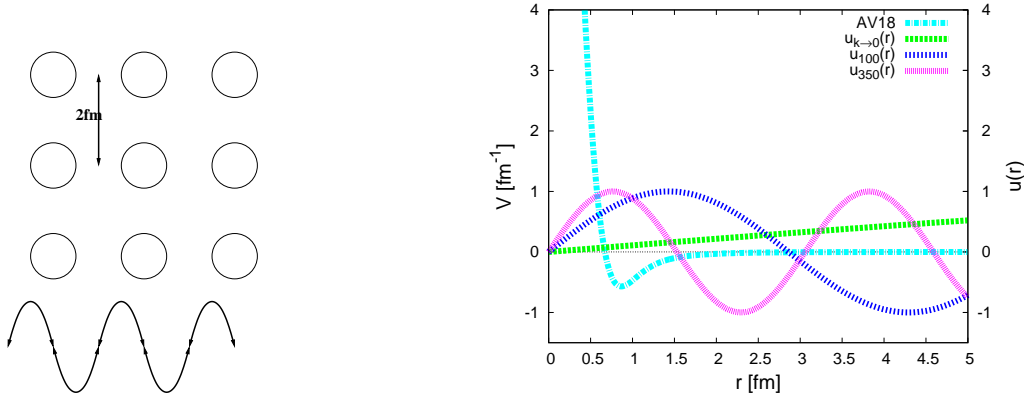


Figure 1: Left panel: Cartoon of a nucleus, displaying the size of the nucleons as compared to the typical distance to nearest neighbors and the shortest wave-lengths wave functions. Right panel: The AV18-potential in the 1S_0 channel. Superposed are the eigen wavefunctions at zero energy, $E_{\text{LAB}} = 100$ MeV and $E_{\text{LAB}} = 350$ MeV.

2 The delta-shells (DS) potential

The basic observation was made long ago by Aviles [7] and recently rediscovered in the context of renormalization of chiral forces [8]. If the two-particle CM wave numbers are limited to a range Δk only gross information can be determined in an interval Δr , (see e.g. Fig. 1) with $\Delta r \Delta k \sim 1$. Thus, for $\Delta k = \Lambda \sim 400 \text{ MeV}$ we have $\Delta r_{\text{min}} \sim 0.5 \text{ fm}$. This uncertainty suggests that for a limited energy range the potential only needs to be known in a limited number of points. With this in mind we consider a neutron-proton (np) potential as a sum of δ functions

$$V(r) = \sum_{i=1}^n \frac{\lambda_i}{2\mu} \delta(r - r_i), \quad (1)$$

where $\mu = M_N/2$ is the reduced np mass of the system, the λ_i coefficients are strength parameters and r_i are the concentration radii. In that case we may determine the s-wave as

$$u(r) = \sin(kr + \delta_{i+1/2}), \quad r_i \leq r \leq r_{i+1}, \quad (2)$$

where $\delta_{i+1/2}(k)$ is the accumulated phase shift at the mid-point $r_{i+1/2}$ and $\delta(k) \equiv \delta_{N+1/2}(k)$. Matching the discontinuity of log-derivatives at $r = r_i$, we simply get

$$k \cot(kr_i + \delta_{i+1/2}) - k \cot(kr_i + \delta_{i-1/2}) = \Delta r U(r_i), \quad (3)$$

where $U(r) = 2\mu V(r) = MV(r)$ is the reduced potential. The regular solution at the origin requires $\delta_{1/2}(k) = 0$. If we take the limit $\Delta r \rightarrow 0$ we can define $\delta(k, r_i) = \delta_i(k)$, to get

$$\frac{d\delta(k, R)}{dR} = -\frac{1}{k} U(R) \sin^2(kR + \delta(k, R)) + \mathcal{O}(\Delta r^2). \quad (4)$$

which is the variable phase equation [9] up to finite grid corrections and can be interpreted as the change in the accumulated phase when a truncated potential of the parametric form $U(r)\theta(R - r)$ is steadily switched on as a function of the variable R . This equation and its generalization to coupled channels has extensively been used to treat the renormalization problem in NN scattering in Refs. [10, 11, 12].

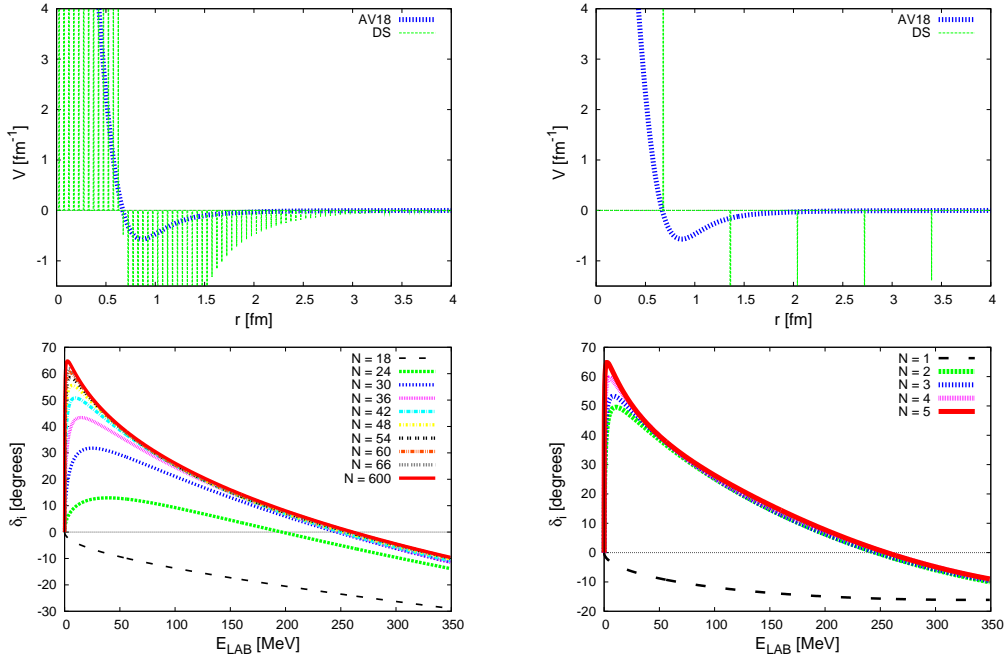


Figure 2: Upper panel: The realistic AV18 potential (1S_0 -channel) and its delta-shell representation (left) and the coarse grained potential (right). Lower panel: Accumulated phase shifts for both cases as a function of the LAB energy (in MeV) indicating the number of grid points. Both resulting phase-shifts coincide.

The low energy expansion of the discrete variable phase equations was used in Ref. [13] to determine threshold parameters in all partial waves. The relation to the well-known Nyquist theorem of sampling a signal with a given bandwidth has been discussed in Ref. [8]. Of course, this DS approximation to the potential can be most immediately used as a numerical method to solve the scattering problem, which would become exact for $\Delta r \rightarrow 0$, if we take the weights *given* by the potential $\lambda_i = U(r_i)\Delta r_i$. As an illustration we show in Fig. 2 the phase-shifts obtained for the 1S_0 -AV18 potential for several values of Δr . Convergence to the phases to four significant figures is achieved for $\Delta r = 0.01\text{fm}$. The equidistant discretization corresponds to the trapezoidal rule and one could improve by a more sophisticated method, a relevant issue when the interaction is known *a priori*.

3 Coarse grained local potentials

Another, more fruitful and economical, perspective already pursued by Aviles corresponds to consider the weights themselves, λ_i , as fitting parameters to the phase-shifts, since anyhow the potential at short distances is unknown and will be determined from the data.

If we take just one delta-shell in S-wave we may determine both the point $r = r_c$ and its corresponding strength, λ_c from the scattering length α_0 and the effective range r_0 , defined from

$$k \cot \delta_0(k) = -\frac{1}{\alpha_0} + \frac{1}{2}r_0k^2 + \dots \quad (5)$$

For instance, for the 1S_0 case one has $\alpha_{0,^1S_0} = -23.74\text{fm}$ and $r_{0,^1S_0} = 2.77\text{fm}$ which yields $\lambda_{1S_0} = -0.4626$ and $r_{c,^1S_0} = 1.99\text{fm}$ whereas for the 3S_1 channel one gets $\alpha_{0,^3S_1} = 5.42\text{fm}$ and $r_{3S_1} = 1.75\text{fm}$ giving $\lambda_{3S_1} = -0.911$ and $r_{c,^3S_1} = 1.53\text{fm}$. The corresponding phase shifts are reproduced to about

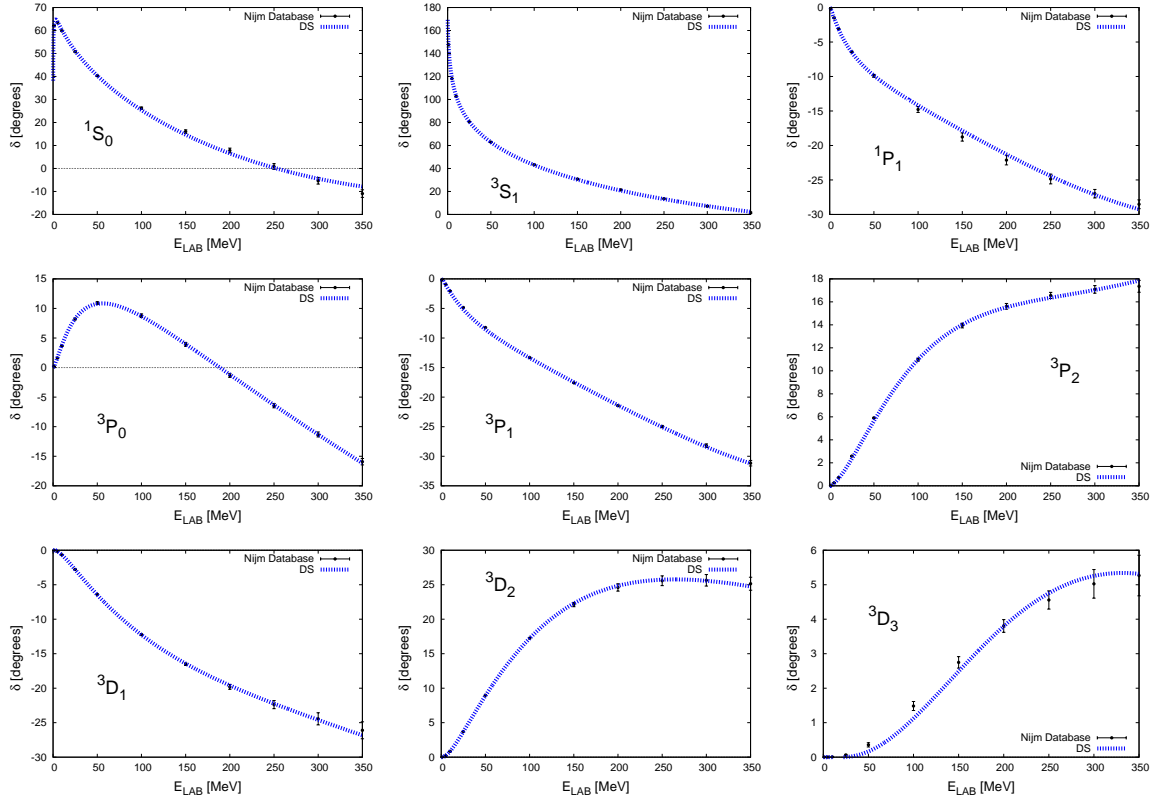


Figure 3: Phase-shifts fitted to the PWA of Nijmegen in the lowest partial waves.

$E_{\text{LAB}} \lesssim 50 \text{ MeV}$. One can improve on this by including more delta-shells. A good fit to the PWA is obtained for (λ_i in fm^{-1} and r_i in fm)

$$\begin{aligned}
 (\lambda_i, r_i) &= (-0.568, 1.56), (-0.023, 3.47), \quad {}^1S_0, \\
 (\lambda_i, r_i) &= (-0.951, 1.35), (-0.052, 2.60), \quad {}^3S_1.
 \end{aligned} \tag{6}$$

This shows that one can consider the grid points as well as the weights as fitting parameters. The result for 5 equidistant points with $\Delta r = 0.7 \text{ fm}$ is shown in Fig. 2 (right panel). Of course, the existence of finite experimental errors helps in decreasing the number of coarse grained grid points.

We have carried out preliminary fits to the NN database [1] with a pion tail with an average $m_\pi = 138 \text{ MeV}$ starting at 2fm for partial waves with $J \leq 4$ and about 40 parameters with $\chi^2/\text{dof} \lesssim 1-2$. The result for low partial waves is shown in Fig. 3. The full PWA using a CD-OPE potential tail with the pertinent electromagnetic corrections to the PWA database will be presented elsewhere.

It is straightforward to look at the deuteron by analysing the ${}^3S_1 - {}^3D_1$ channel for negative energy. The results can be seen in Table 1. The deuteron wave functions as well as the corresponding charge form factor is displayed in Fig. 4. The peaks in the wave functions correspond to the discontinuity in the derivatives at the chosen grid points which, as we can see, does not become dramatic for the form factor at the considered q 's.

Fourier transforming the DS potential in the S-waves gives

$$\langle k' | V_{il}^{SJ} | k \rangle = \sum_i (\lambda_i)_{il}^{SJ} r_i^2 j_{l'}(k' r_i) j_l(k r_i), \tag{7}$$

which is a finite rank separable potential, a representation which proved very handy in the past for few-body and nuclear matter calculations (see e.g. [14]).

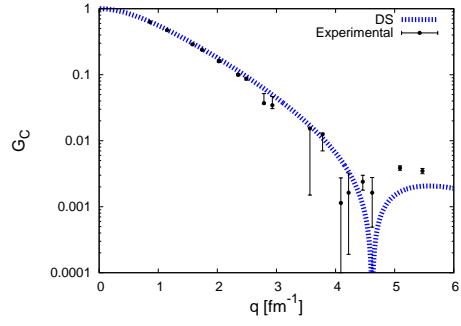
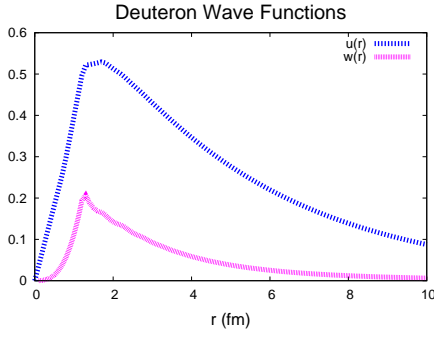


Figure 4: Left panel: The deuteron wave functions Right panel: Charge form factor.

Table 1: Deuteron parameters

	Delta Shell	Empirical	Nijm I [2]	Nijm II [2]	Reid93 [2]	AV18 [3]
$\gamma(\text{fm}^{-1})$	0.230348	0.231605	Input	Input	Input	Input
η	0.02488	0.0256(5)	0.02534	0.02521	0.02514	0.0250
$A_S(\text{fm}^{1/2})$	0.8768	0.8781(44)	0.8841	0.8845	0.8853	0.8850
$r_m(\text{fm})$	1.9676	1.953(3)	1.9666	1.9675	1.9686	1.967
$Q_D(\text{fm}^2)$	0.2693	0.2859(3)	0.2719	0.2707	0.2703	0.270
P_D	5.498	5.67(4)	5.664	5.635	5.699	5.76

We show in Fig. 5 a comparison of the Fourier transformed DS potentials in the 1S_0 and 3S_1 channels with with parameters as in Eq. (6) to the corresponding diagonal elements of the V_{lowk} potentials [5], obtained from the AV18 [3] interaction. While the resemblance is indeed rather close, we do not expect a perfect description since the way the scattering problem is treated in the DS case is *different* as in the V_{lowk} case. We have checked that one can represent quite accurately the current diagonal pieces of the V_{lowk} potentials [5] by Eq. (7), but does not necessarily reproduce the off-diagonal matrix elements constructed in the V_{lowk} approach from the truncated the half-off shell Lippmann-Schwinger equation by a specific block-transformation method.

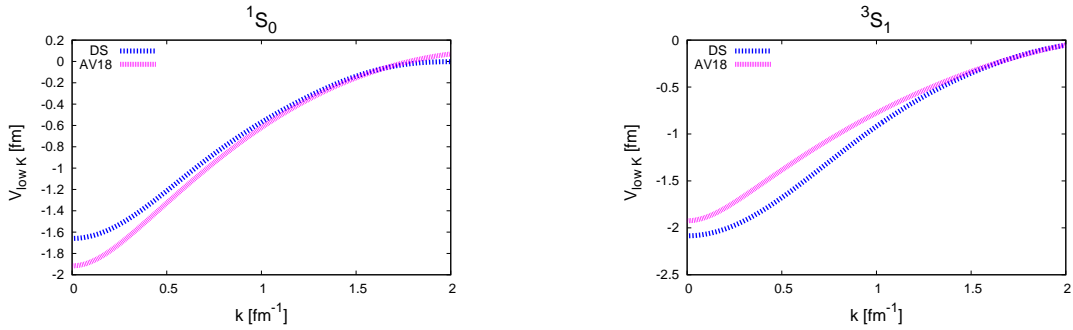


Figure 5: Comparison of the coordinate space coarse-grained potentials in the 1S_0 and 3S_1 channels with the corresponding V_{lowk} potentials [5], obtained from the AV18 [3] interaction.

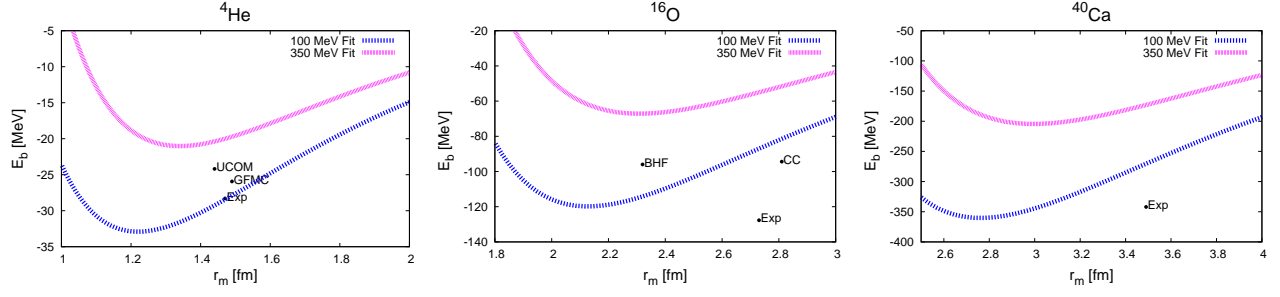


Figure 6: Binding energy of closed-shell nuclei ${}^4\text{He}$, ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$ using a HO shell model Slater determinant as a function of the msr when the relevant phase shifts are reproduced up to $E_{\text{LAB}} = 100\text{MeV}$ and $E_{\text{LAB}} = 350\text{MeV}$. We compare to other methods (see main text).

4 Closed-shell nuclei

When switching from the NN problem to the many body nuclear problem the features and the form of the interaction are relevant in terms of computational cost and feasibility. We coarse-grain the interaction, but keep the exact kinetic energy, so that for two nucleons at a relative distance $|\vec{x}_1 - \vec{x}_2| \neq r_c$ the interaction vanishes, and hence the wave function becomes a Slater determinant of single particle states

$$\psi(\vec{x}_1, \dots, \vec{x}_A) = \mathcal{A} [\phi_{n_1, l_1, s, m_{s1}, t, m_{t1}}(\vec{x}_1) \dots \phi_{n_A, l_A, s, m_{sA}, t, m_{tA}}(\vec{x}_A)] . \quad (8)$$

We use Harmonic Oscillator single particle wave functions with oscillator parameter b , where the spurious CM motion is exactly subtracted, for the shell-configurations ${}^4\text{He}:(1s)^4$, ${}^{16}\text{O}:(1s)^4(1p)^{12}$ and ${}^{40}\text{Ca}:(1s)^4(1p)^{12}(2s)^4(1d)^{20}$. Generally, for double-closed shell nuclei one has

$$\langle V_2 \rangle_A = \sum_{nlJS} g_{nlJS} \langle nl | V^{JST} | nl \rangle , \quad (9)$$

in terms of the relative matrix elements and g_{nljs} depends on the Talmi-Moshinsky brackets¹. Using the single delta function which is just fixed with the S-waves scattering lengths and effective ranges (see below Eq. (5)) one obtains at the minimum $B({}^4\text{He}) = 20\text{MeV}$. In common with other soft potentials [6] the interaction does not require strong correlations in the many-body wave function. This is due to the fact that since the phase-shift is reproduced to about $E_{\text{LAB}} = 50\text{MeV}$ the core may be ignored. Clearly, if we insist on reproducing up to $E_{\text{LAB}} = 350\text{MeV}$ a strongly repulsive DS contribution emerges and thus a product wave function is not appropriate. One can improve on this by adding more deltas as in Eq. (6) but keeping the fit to $E_{\text{LAB}} \leq 100\text{MeV}$, in which case $B({}^4\text{He}) = 24\text{MeV}$. This is surprisingly close to the Green Function Monte Carlo (GFMC) AV18 [4] and the UCOM method [15] without three-body forces and complies to a cancellation between the core in the and the correlations the wave function.

The results for the binding energy as a function of the corresponding msr radius are presented in Fig. 6. We compare with the UCOM method [15], Brueckner-Hartree-Fock (BHF) [16] and Coupled Cluster (CC) [17]. In the UCOM method [15] a unitary local transformation generates a smooth nonlocal interaction from the AV18-potential while the wave functions are the same. As advertised, our results depend on the fitted energy range, somewhat resembling analogous ambiguities as those of the UCOM.

¹For instance, for ${}^4\text{He}$ one has a m.s.r. $r_m = 3b/2\sqrt{2}$ and for $R_{1s}(r) = 2e^{-\frac{r^2}{2b^2}} / \sqrt[4]{\pi} b^{3/2}$,

$$\langle T \rangle_{{}^4\text{He}} + \langle V_2 \rangle_{{}^4\text{He}} = 3 \langle 1s | \frac{p^2}{2M} | 1s \rangle + 6 \langle 1s | \frac{1}{2} (V_{1S_0} + V_{3S_1}) | 1s \rangle = \frac{9}{4b^2M} + \frac{6}{b^3M} \sqrt{\frac{2}{\pi}} \sum_n (\lambda_{n,1S_0} + \lambda_{n,3S_1}) r_n^2 e^{-\frac{r_n^2}{2b^2}}$$

For an Android implementation of these calculations see e.g. <http://www.ugr.es/~amaro/android/>

5 Conclusions

We have shown how sampling of the NN interaction by a delta shell potential with a resolution determined by the deBroglie wavelength of the most energetic particle provides a coarse graining in configuration space, analogous to the V_{lowk} approach. However, rather than transforming a high quality potential we suggest to determine the NN coarse grained interaction directly from the scattering data. A preliminary fit to the np phase shifts in the Nijmegen data base to all partial waves with $j \leq 4$ requires about 40 fitting parameters yielding $\chi^2/\text{d.o.f.} \lesssim 2$ (less than 1 in some waves). Deuteron properties show good agreement with empirical values and other calculations. Harmonic oscillator shell model variational calculations of nuclear binding energies provide results at the 20-30% accuracy.

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References

- [1] V.G.J. Stoks, R.A.M. Kompl, M.C.M. Rentmeester, and J.J. de Swart. *Phys.Rev.*, C48:792–815, 1993.
- [2] V.G.J. Stoks, R.A.M. Klomp, C.P.F. Terheggen, and J.J. de Swart. *Phys.Rev.*, C49:2950–2962, 1994.
- [3] Robert B. Wiringa, V.G.J. Stoks, and R. Schiavilla. *Phys.Rev.*, C51:38–51, 1995.
- [4] Steven C. Pieper and Robert B. Wiringa. *Ann.Rev.Nucl.Part.Sci.*, 51:53–90, 2001.
- [5] S.K. Bogner, T.T.S. Kuo, and A. Schwenk. *Phys.Rept.*, 386:1–27, 2003.
- [6] I.R. Afnan and Y.C. Tang. *Phys.Rev.*, 175:1337–1345, 1968.
- [7] J.B. Aviles. *Phys.Rev.*, C6:1467–1484, 1972.
- [8] D.R. Entem, E. Ruiz Arriola, M. Pavon Valderrama, and R. Machleidt. *Phys.Rev.*, C77:044006, 2008.
- [9] F. Calogero. *Variable Phase Approach to Potential Scattering*. Academic Press, New York, 1967.
- [10] M. Pavon Valderrama and E. Ruiz Arriola. *Phys. Lett.*, B580:149–156, 2004.
- [11] M. Pavon Valderrama and E. Ruiz Arriola. *Phys. Rev.*, C70:044006, 2004.
- [12] M. Pavon Valderrama and E. Ruiz Arriola. *Annals Phys.*, 323:1037–1086, 2008.
- [13] M. Pavon Valderrama and E. Ruiz Arriola. *Phys.Rev.*, C72:044007, 2005.
- [14] P. Grygorov, E.N.E. van Dalen, H. Muther, and J. Margueron. *Phys.Rev.*, C82:014315, 2010.
- [15] Thomas Neff and Hans Feldmeier. *Nucl.Phys.*, A713:311–371, 2003.
- [16] H. Muther and A. Polls. *Prog.Part.Nucl.Phys.*, 45:243–334, 2000.
- [17] Jochen H. Heisenberg and Bogdan Mihaila. *Phys.Rev.*, C59:1440–1448, 1999.